



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:12 PM UTC

PDB ID : 7QOV / pdb_00007qov
Title : The wild type nitrile hydratase from *Geobacillus pallidus*
Authors : Van Wyk, J.C.; Cowan, D.A.; Danson, M.J.; Tsekoa, T.L.; Sayed, M.F.; Sewell, B.T.
Deposited on : 2021-12-29
Resolution : 1.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

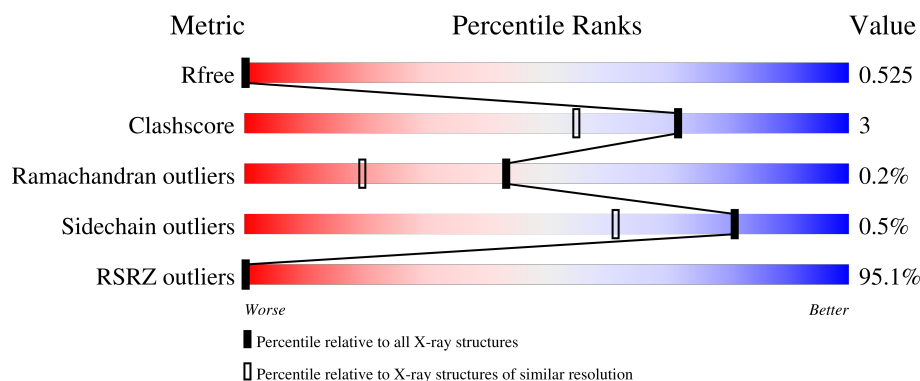
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	90% 85% 7% 6%
2	B	229	92% 88% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3988 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nitrile hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	2	0
			1641	1046	284	303	8			

- Molecule 2 is a protein called Nitrile hydratase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	4	0
			1876	1210	314	343	9			

- Molecule 3 is COBALT (III) ION (CCD ID: 3CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	2	Total	Cl	0	0
			2	2		

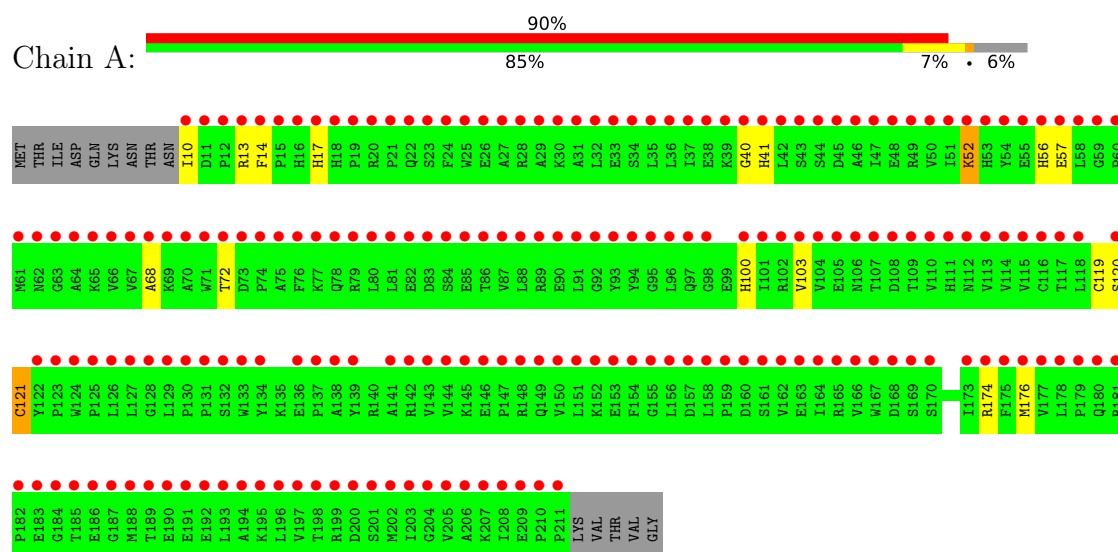
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	212	Total	O	0	0
			212	212		
5	B	255	Total	O	0	0
			255	255		

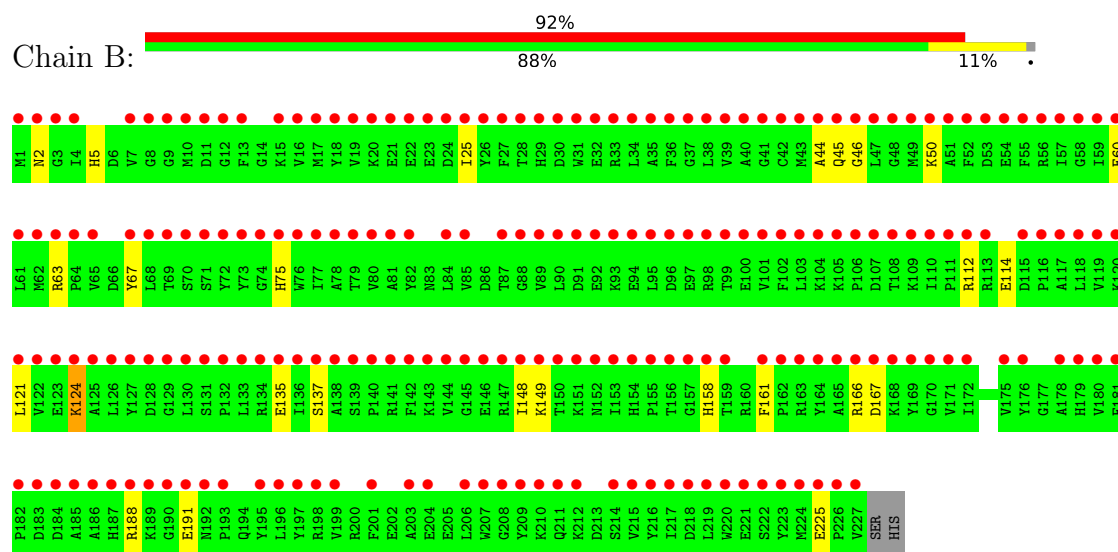
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Nitrile hydratase



• Molecule 2: Nitrile hydratase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.48Å 105.48Å 83.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.59 – 1.40 27.59 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.59-1.40) 87.4 (27.59-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.50 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.10.1	Depositor
R, R_{free}	(Not available) , 0.180 0.542 , 0.525	Depositor DCC
R_{free} test set	5083 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 21.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	3988	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3CO, CSD, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/1676	0.66	0/2279
2	B	0.47	0/1940	0.68	0/2620
All	All	0.45	0/3616	0.67	0/4899

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1641	0	1627	8	9
2	B	1876	0	1843	15	14
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	1	0
5	A	212	0	0	3	13
5	B	255	0	0	7	20
All	All	3988	0	3470	23	31

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ASN:HD21	2:B:166:ARG:HH12	1.24	0.84
2:B:225:GLU:HG2	5:B:561:HOH:O	1.92	0.69
2:B:60:GLU:OE1	2:B:158:HIS:HD2	1.81	0.63
1:A:72[B]:THR:HG23	5:A:420:HOH:O	2.03	0.57
2:B:75:HIS:HD2	5:B:615:HOH:O	1.87	0.57
2:B:158:HIS:HE1	5:B:459:HOH:O	1.88	0.55
2:B:67:TYR:O	2:B:75:HIS:HE1	1.90	0.55
1:A:121:CSD:HB2	1:A:174:ARG:CZ	2.38	0.52
1:A:14:PHE:HB3	1:A:17:HIS:CD2	2.45	0.51
2:B:124:LYS:NZ	5:B:402:HOH:O	2.43	0.50
1:A:100:HIS:HD2	5:A:567:HOH:O	1.95	0.49
2:B:121:LEU:HD23	2:B:121:LEU:C	2.37	0.49
2:B:149:LYS:HE2	2:B:167:ASP:OD1	2.13	0.49
2:B:5:HIS:HD2	5:B:497:HOH:O	1.97	0.48
2:B:225:GLU:CG	5:B:561:HOH:O	2.55	0.47
2:B:225:GLU:CD	5:B:561:HOH:O	2.58	0.47
1:A:17:HIS:HD2	5:A:586:HOH:O	1.98	0.45
1:A:68:ALA:O	1:A:72[B]:THR:HG22	2.17	0.44
2:B:63:ARG:HD2	4:B:302:CL:CL	2.54	0.43
1:A:103:VAL:HG22	1:A:176[B]:MET:HE2	2.00	0.42
2:B:148:ILE:HD12	2:B:148:ILE:C	2.44	0.42
1:A:52:LYS:HB2	1:A:52:LYS:NZ	2.35	0.41
2:B:161:PHE:CZ	2:B:166:ARG:HG2	2.56	0.40

All (31) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:568:HOH:O	5:B:431:HOH:O[8_777]	0.97	1.23
5:A:593:HOH:O	5:B:603:HOH:O[3_745]	1.25	0.95
5:B:606:HOH:O	5:B:612:HOH:O[4_574]	1.41	0.79
1:A:57:GLU:OE2	5:A:603:HOH:O[3_745]	1.59	0.61
2:B:188:ARG:O	5:B:536:HOH:O[4_574]	1.62	0.58
5:B:455:HOH:O	5:B:643:HOH:O[8_777]	1.68	0.52
5:B:534:HOH:O	5:B:583:HOH:O[4_574]	1.68	0.52
2:B:25[A]:ILE:CG2	5:B:513:HOH:O[3_745]	1.69	0.51
2:B:114:GLU:OE2	5:B:408:HOH:O[3_745]	1.69	0.51
2:B:25[B]:ILE:CG2	5:B:513:HOH:O[3_745]	1.74	0.46
2:B:135:GLU:OE2	5:B:629:HOH:O[4_574]	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:578:HOH:O	5:B:655:HOH:O[3_745]	1.79	0.41
5:A:427:HOH:O	5:A:583:HOH:O[4_574]	1.80	0.40
5:A:468:HOH:O	5:B:496:HOH:O[3_745]	1.81	0.39
5:A:471:HOH:O	5:B:538:HOH:O[8_777]	1.82	0.38
1:A:56:HIS:CD2	2:B:45:GLN:O[3_745]	1.98	0.22
1:A:10:ILE:O	2:B:137:SER:N[5_747]	2.01	0.19
1:A:56:HIS:CD2	2:B:45:GLN:C[3_745]	2.01	0.19
5:B:517:HOH:O	5:B:596:HOH:O[4_574]	2.01	0.19
2:B:45:GLN:OE1	5:A:472:HOH:O[4_574]	2.03	0.17
2:B:191:GLU:N	5:B:557:HOH:O[4_574]	2.05	0.15
5:A:476:HOH:O	5:B:450:HOH:O[3_745]	2.07	0.13
5:A:537:HOH:O	5:B:456:HOH:O[5_747]	2.07	0.13
5:A:485:HOH:O	5:B:466:HOH:O[5_747]	2.10	0.10
1:A:13:ARG:CG	5:B:612:HOH:O[8_777]	2.13	0.07
1:A:40:GLY:O	5:A:606:HOH:O[4_574]	2.13	0.07
2:B:50:LYS:NZ	5:A:454:HOH:O[4_574]	2.14	0.06
2:B:112:ARG:NE	5:B:541:HOH:O[3_745]	2.15	0.05
1:A:41:HIS:CE1	5:A:402:HOH:O[4_574]	2.17	0.03
1:A:56:HIS:ND1	2:B:44:ALA:O[3_745]	2.18	0.02
1:A:56:HIS:NE2	2:B:46:GLY:N[3_745]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/216 (93%)	194 (97%)	5 (2%)	1 (0%)	24	7
2	B	228/229 (100%)	223 (98%)	5 (2%)	0	100	100
All	All	428/445 (96%)	417 (97%)	10 (2%)	1 (0%)	43	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/190 (94%)	178 (99%)	1 (1%)	78	56
2	B	198/196 (101%)	197 (100%)	1 (0%)	81	61
All	All	377/386 (98%)	375 (100%)	2 (0%)	81	61

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
2	B	124	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
2	B	2	ASN
2	B	5	HIS
2	B	75	HIS
2	B	152	ASN
2	B	158	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	A	119	1	4,7,8	6.41	1 (25%)	1,8,10	0.17	0
1	CSD	A	121	3,1	4,7,8	8.39	1 (25%)	1,8,10	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	119	1	-	0/2/6/8	-
1	CSD	A	121	3,1	-	0/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	CSD	OD1-SG	16.73	1.62	1.47
1	A	119	CSD	OD1-SG	12.77	1.59	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	121	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	200/216 (92%)	4.48	195 (97%) 0 0	8, 12, 24, 33	3 (1%)
2	B	227/229 (99%)	4.33	211 (92%) 0 0	7, 11, 25, 32	5 (2%)
All	All	427/445 (95%)	4.40	406 (95%) 0 0	7, 12, 25, 33	8 (1%)

All (406) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	GLY	13.1
1	A	211	PRO	12.1
2	B	103	LEU	10.6
2	B	101	VAL	10.1
2	B	110	ILE	10.0
2	B	116	PRO	9.4
2	B	122	VAL	9.2
1	A	124	TRP	9.0
2	B	89	VAL	8.8
1	A	32	LEU	8.6
1	A	98	GLY	8.5
1	A	210	PRO	8.5
1	A	76	PHE	8.4
2	B	106	PRO	8.4
1	A	129	LEU	8.3
2	B	47[A]	LEU	8.3
2	B	217	ILE	8.2
1	A	91	LEU	8.1
1	A	10	ILE	7.8
2	B	72	TYR	7.8
1	A	47	ILE	7.8
1	A	193	LEU	7.6
2	B	161	PHE	7.6
1	A	110	VAL	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	21	PRO	7.3
2	B	227	VAL	7.2
1	A	197	VAL	7.1
2	B	16	VAL	7.1
1	A	71	TRP	7.1
2	B	144	VAL	7.0
1	A	12	PRO	6.9
2	B	102	PHE	6.9
2	B	220	TRP	6.9
2	B	27	PHE	6.8
1	A	154	PHE	6.8
2	B	105	LYS	6.8
1	A	208	ILE	6.7
1	A	189	THR	6.7
1	A	184	GLY	6.7
2	B	92	GLU	6.7
2	B	133	LEU	6.7
2	B	117	ALA	6.6
2	B	153	ILE	6.6
1	A	25	TRP	6.6
1	A	205	VAL	6.5
1	A	158	LEU	6.5
2	B	109	LYS	6.5
2	B	150	THR	6.4
1	A	87	VAL	6.4
1	A	78	GLN	6.4
2	B	223	TYR	6.4
2	B	25[A]	ILE	6.3
2	B	136	ILE	6.3
2	B	171	VAL	6.3
2	B	18	TYR	6.3
1	A	56	HIS	6.2
2	B	169	TYR	6.2
2	B	104	LYS	6.2
1	A	79	ARG	6.2
2	B	118	LEU	6.2
2	B	19	VAL	6.1
2	B	178	ALA	6.1
2	B	175	VAL	6.1
1	A	127	LEU	6.0
1	A	156	LEU	6.0
1	A	157	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	24	PHE	6.0
2	B	142	PHE	6.0
1	A	206	ALA	6.0
2	B	90	LEU	5.9
1	A	150	VAL	5.9
1	A	93	TYR	5.9
1	A	115	VAL	5.9
2	B	158	HIS	5.9
2	B	31	TRP	5.8
2	B	156	THR	5.8
1	A	62	ASN	5.8
2	B	121	LEU	5.8
1	A	207	LYS	5.8
2	B	127	TYR	5.8
2	B	108	THR	5.8
2	B	193	PRO	5.7
1	A	144	VAL	5.7
2	B	65	VAL	5.7
1	A	86	THR	5.7
2	B	4	ILE	5.7
1	A	80	LEU	5.7
2	B	219	LEU	5.7
2	B	215	VAL	5.7
1	A	190	GLU	5.7
2	B	111	PRO	5.6
1	A	94	TYR	5.6
2	B	73	TYR	5.6
1	A	143	VAL	5.6
1	A	166	VAL	5.6
2	B	34	LEU	5.6
2	B	84	LEU	5.5
2	B	170	GLY	5.5
1	A	58	LEU	5.5
1	A	61	MET	5.5
2	B	157	GLY	5.5
2	B	124	LYS	5.5
2	B	82	TYR	5.4
2	B	216	TYR	5.4
1	A	75	ALA	5.4
1	A	68	ALA	5.4
2	B	148	ILE	5.3
2	B	167	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	55	PHE	5.3
2	B	23	GLU	5.3
1	A	173	ILE	5.3
2	B	128	ASP	5.3
1	A	151	LEU	5.3
1	A	126	LEU	5.3
2	B	196	LEU	5.3
2	B	85	VAL	5.3
2	B	68	LEU	5.2
2	B	119	VAL	5.2
1	A	123	PRO	5.2
1	A	36	LEU	5.2
2	B	210	LYS	5.2
1	A	163	GLU	5.2
1	A	196	LEU	5.2
2	B	195	TYR	5.1
2	B	96	ASP	5.1
2	B	12	GLY	5.1
2	B	207	TRP	5.1
2	B	24	ASP	5.1
1	A	90	GLU	5.1
1	A	83	ASP	5.0
2	B	199	VAL	5.0
2	B	13	PHE	5.0
2	B	209	TYR	5.0
2	B	20	LYS	5.0
2	B	76	TRP	5.0
1	A	114	VAL	5.0
2	B	69	THR	5.0
2	B	99	THR	5.0
1	A	209	GLU	5.0
1	A	175	PHE	5.0
2	B	155	PRO	4.9
1	A	160	ASP	4.9
1	A	63	GLY	4.9
1	A	67	VAL	4.9
2	B	190	GLY	4.9
1	A	202	MET	4.9
1	A	182	PRO	4.9
1	A	104	VAL	4.9
2	B	61	LEU	4.8
1	A	92	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	72[A]	THR	4.8
1	A	194	ALA	4.8
2	B	64	PRO	4.8
1	A	159	PRO	4.8
2	B	11	ASP	4.7
2	B	52	PHE	4.7
2	B	57	ILE	4.7
2	B	212	LYS	4.7
2	B	26	TYR	4.7
1	A	19	PRO	4.7
2	B	113	ARG	4.7
1	A	185	THR	4.6
1	A	28	ARG	4.6
1	A	18	HIS	4.6
2	B	125	ALA	4.6
2	B	143	LYS	4.6
2	B	98	ARG	4.6
1	A	81	LEU	4.6
1	A	103	VAL	4.6
2	B	94	GLU	4.6
1	A	147	PRO	4.6
1	A	96	LEU	4.6
1	A	46	ALA	4.6
1	A	54	TYR	4.6
2	B	43	MET	4.6
2	B	172	ILE	4.5
2	B	9	GLY	4.5
1	A	130	PRO	4.5
2	B	164	TYR	4.5
1	A	53	HIS	4.5
1	A	73	ASP	4.5
1	A	133	TRP	4.5
1	A	88	LEU	4.5
2	B	95	LEU	4.5
2	B	185	ALA	4.5
1	A	188	MET	4.5
1	A	164	ILE	4.4
2	B	107	ASP	4.4
2	B	206	LEU	4.4
1	A	65	LYS	4.4
1	A	82	GLU	4.4
2	B	138	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	188	ARG	4.4
1	A	139	TYR	4.4
2	B	39	VAL	4.4
2	B	15[A]	LYS	4.3
1	A	149	GLN	4.3
1	A	35	LEU	4.3
1	A	203	ILE	4.3
2	B	77	ILE	4.3
1	A	179	PRO	4.3
1	A	128	GLY	4.3
2	B	181	PHE	4.3
1	A	134	TYR	4.3
1	A	162	VAL	4.3
1	A	195	LYS	4.3
1	A	101	ILE	4.3
1	A	15	PRO	4.2
1	A	155	GLY	4.2
2	B	137	SER	4.2
2	B	45	GLN	4.2
1	A	113	VAL	4.2
2	B	91	ASP	4.2
1	A	138	ALA	4.2
1	A	51	ILE	4.2
1	A	40	GLY	4.2
1	A	199	ARG	4.2
1	A	42	LEU	4.2
2	B	50	LYS	4.2
1	A	70	ALA	4.2
2	B	112	ARG	4.2
2	B	197	TYR	4.2
1	A	27	ALA	4.2
1	A	84	SER	4.1
2	B	126	LEU	4.1
2	B	130	LEU	4.1
2	B	35	ALA	4.1
1	A	66	VAL	4.1
1	A	198	THR	4.1
1	A	131	PRO	4.1
2	B	36	PHE	4.1
2	B	70	SER	4.1
1	A	168	ASP	4.1
1	A	161	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	141	ALA	4.1
2	B	176	TYR	4.1
2	B	163	ARG	4.0
2	B	29	HIS	4.0
1	A	64	ALA	4.0
1	A	59	GLY	4.0
1	A	118	LEU	4.0
2	B	203	ALA	4.0
1	A	31	ALA	4.0
2	B	17	MET	4.0
1	A	39	LYS	3.9
1	A	77	LYS	3.9
1	A	120	SER	3.9
1	A	204	GLY	3.9
1	A	50	VAL	3.9
2	B	51	ALA	3.9
1	A	183	GLU	3.9
2	B	7	VAL	3.9
2	B	49	MET	3.9
1	A	14	PHE	3.8
1	A	69	LYS	3.8
2	B	28	THR	3.8
1	A	38	GLU	3.8
2	B	22	GLU	3.8
2	B	187	HIS	3.8
1	A	122	TYR	3.7
2	B	186	ALA	3.7
1	A	41	HIS	3.7
2	B	211	GLN	3.7
2	B	147	ARG	3.7
1	A	74	PRO	3.7
1	A	17	HIS	3.7
2	B	179	HIS	3.7
2	B	180	VAL	3.7
1	A	191	GLU	3.7
1	A	152	LYS	3.7
2	B	40	ALA	3.7
1	A	186	GLU	3.6
1	A	178	LEU	3.6
1	A	37	ILE	3.6
1	A	181	ARG	3.6
2	B	41	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	48	GLU	3.6
1	A	176[A]	MET	3.6
2	B	80	VAL	3.6
2	B	151	LYS	3.6
2	B	139	SER	3.6
2	B	120	LYS	3.6
2	B	21	GLU	3.5
2	B	97	GLU	3.5
2	B	204	GLU	3.5
2	B	165	ALA	3.5
2	B	198	ARG	3.5
2	B	8	GLY	3.5
2	B	88	GLY	3.5
1	A	106	ASN	3.5
1	A	167	TRP	3.5
2	B	182	PRO	3.5
2	B	87	THR	3.5
2	B	168	LYS	3.5
1	A	137	PRO	3.5
1	A	177	VAL	3.5
2	B	78	ALA	3.4
2	B	123	GLU	3.4
1	A	112	ASN	3.4
2	B	184	ASP	3.4
1	A	125	PRO	3.4
1	A	153	GLU	3.4
1	A	192	GLU	3.4
2	B	58	GLY	3.4
2	B	100	GLU	3.4
2	B	93	LYS	3.3
2	B	79	THR	3.3
2	B	59	ILE	3.3
2	B	145	GLY	3.3
2	B	1[A]	MET	3.3
2	B	141	ARG	3.3
1	A	60	PRO	3.3
2	B	140	PRO	3.2
1	A	13	ARG	3.2
2	B	74	GLY	3.2
1	A	23	SER	3.2
1	A	132	SER	3.2
2	B	38	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	33	GLU	3.2
1	A	97	GLN	3.1
2	B	132	PRO	3.1
1	A	44	SER	3.1
2	B	214	SER	3.1
1	A	30	LYS	3.1
1	A	201	SER	3.1
2	B	81	ALA	3.1
1	A	34	SER	3.0
1	A	200	ASP	3.0
2	B	201	PHE	3.0
2	B	149	LYS	3.0
2	B	46	GLY	3.0
1	A	107	THR	3.0
2	B	135	GLU	2.9
2	B	225	GLU	2.9
2	B	71	SER	2.9
1	A	146	GLU	2.9
2	B	134	ARG	2.9
2	B	159	THR	2.9
1	A	148	ARG	2.9
1	A	145	LYS	2.9
2	B	10	MET	2.9
1	A	89	ARG	2.9
1	A	165	ARG	2.9
2	B	2	ASN	2.9
2	B	152	ASN	2.9
1	A	11	ASP	2.8
2	B	131	SER	2.8
2	B	42	CYS	2.8
2	B	146	GLU	2.8
2	B	37	GLY	2.8
1	A	55	GLU	2.8
1	A	16	HIS	2.8
2	B	221	GLU	2.8
2	B	154	HIS	2.8
1	A	22	GLN	2.7
1	A	95	GLY	2.7
2	B	222	SER	2.7
2	B	56	ARG	2.7
1	A	116	CYS	2.7
2	B	48	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	30	ASP	2.6
2	B	226	PRO	2.6
1	A	52	LYS	2.6
1	A	111	HIS	2.6
2	B	75	HIS	2.6
1	A	20	ARG	2.6
1	A	49	ARG	2.6
1	A	109	THR	2.6
2	B	189	LYS	2.6
2	B	191	GLU	2.6
2	B	53	ASP	2.6
2	B	208	GLY	2.6
1	A	169	SER	2.6
2	B	115	ASP	2.5
2	B	54	GLU	2.5
2	B	162	PRO	2.5
1	A	29	ALA	2.5
1	A	170	SER	2.4
2	B	192	ASN	2.4
1	A	43	SER	2.4
2	B	166	ARG	2.4
2	B	67	TYR	2.4
2	B	218	ASP	2.4
1	A	142	ARG	2.4
2	B	63	ARG	2.4
1	A	180	GLN	2.3
2	B	3	GLY	2.3
1	A	108	ASP	2.3
1	A	105	GLU	2.3
2	B	129	GLY	2.3
2	B	32	GLU	2.3
2	B	44	ALA	2.2
2	B	224	MET	2.2
2	B	60	GLU	2.2
1	A	26	GLU	2.2
2	B	62	MET	2.2
2	B	33	ARG	2.2
1	A	45	ASP	2.2
1	A	100	HIS	2.1
1	A	85	GLU	2.1
1	A	102	ARG	2.1
1	A	136	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	117	THR	2.0
1	A	174	ARG	2.0
1	A	57	GLU	2.0
2	B	183	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	121	8/9	0.79	0.20	8,9,11,13	0
1	CSD	A	119	8/9	0.83	0.15	8,9,9,11	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

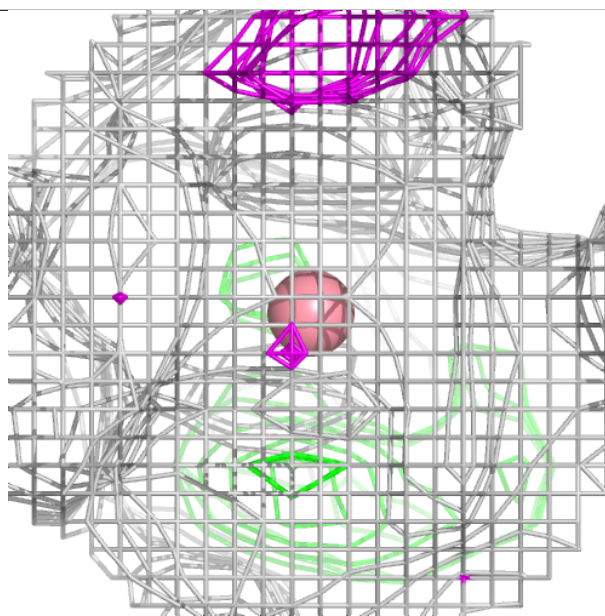
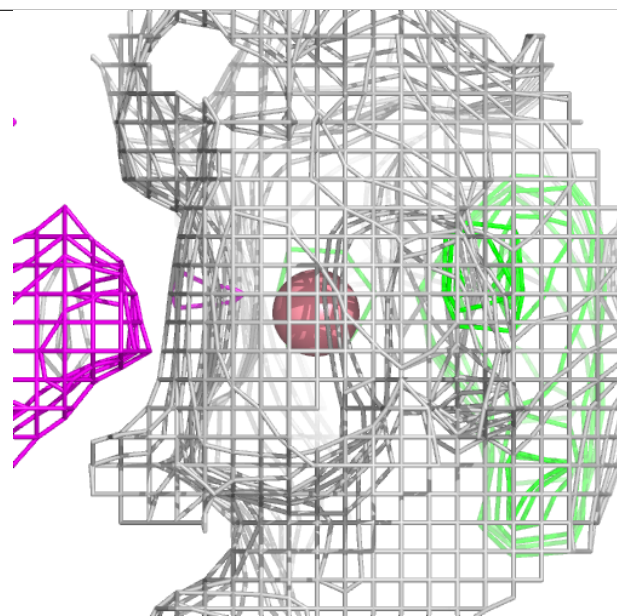
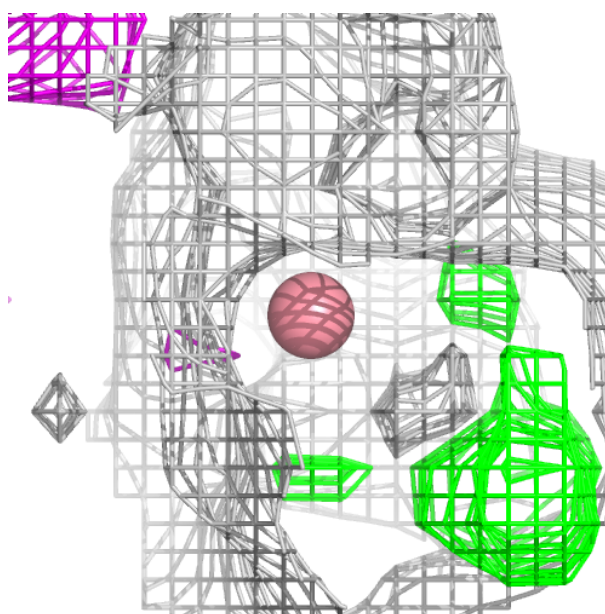
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	B	301	1/1	0.60	0.16	29,29,29,29	0
4	CL	A	302	1/1	0.72	0.24	13,13,13,13	0
4	CL	B	302	1/1	0.87	0.10	24,24,24,24	0
3	3CO	A	301	1/1	0.95	0.07	8,8,8,8	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 3CO A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.